What is claimed is:

1. A computer-aided method for the provision, identification and description of molecules exhibiting a desired behaviour, employing a molecular modelling step, a combinatorial library building step and a step of selecting potentially useful molecules, wherein said method includes a step whereby the candidate molecules are filtered using a using at least one static filter representing a plurality of descriptors and or using at least one dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said activity.

2. A computer-aided method for the provision, identification and description of molecules exhibiting a desired behaviour according to claim 1, wherein it includes a preliminary step of static filtering to reduce the number of candidate molecules and for a subsequent dynamic filtration step.

3. A computer-aided method of designing molecules exhibiting a desired activity, the method comprising the following steps:

1) producing a learning set of molecules including molecules known to exhibit the activity ("active molecules") and molecules known not to exhibit the activity ("inactive molecules");

2) determining the values of a plurality of descriptors of said learning set of molecules;

3) from said values deriving one or more criteria associating descriptor values with activity, said criteria including at least one static criterion and at least one dynamic criterion;

4) generating a plurality of candidate molecules;

5) subjecting the candidate molecules to said static criteria, and disregarding candidate molecules which do not meet said static criteria;

6) subjecting the candidate molecules to said dynamic criterion, and disregarding candidate molecules which do not meet said dynamic criteria;

7) synthesising and testing the remaining candidate molecules to determine whether said remaining candidate molecules are active.

4. A computer-aided method for designing molecules according to claim 3 wherein it further comprises the step:

screening the candidate molecules on the basis of enrichment in molecular diversity terms provided by each molecule in relation to the selected descriptors.

5. A computer-aided method according to claim 3, wherein at least one of said criteria is based on a non-linear function of a descriptor value.

6. A computer-aided method according to claim 3,

wherein said derivation of the criteria includes a step of determining whether at least two criteria have a correlation measured over the learning set above a predetermined value, and if so rejecting at least one of said at least two criteria.

7. A computer-aided method for the provision according to claim 3 , wherein if the desired result is not obtained, or if it is only partly obtained, steps 3 to 7 are repeated, using the inactive synthesised molecules as additional inactive molecules of the learning set.

8. A computer-aided method according to claim 3, wherein at least one of said dynamic criteria is based on the conformational spaces of a candidate molecule.

9. A computer-aided method according to claim 3, wherein at least one of said dynamic criteria is based on a shape descriptor derived from a 3D autocorrelation vector (3D-ACV) of the candidate molecule.

10. A computer-aided method according to claim 3, wherein the static criteria are based on physicochemical and topological descriptors at least some of which are chosen from the descriptors cited in Table II.

11. A computer-aided method for the provision, identification and description of molecules exhibiting a

desired behaviour, according to claim 7, wherein step 7 includes calculating for a candidate molecule a set of 3D-ACV for each of a series of conformations obtained by molecular dynamics (MD) and then treating the 3D-ACV using the multivariate statistics in three main steps (i to iii):

(i) for a given conformation of the molecule being investigated, the corresponding 3D-ACV descriptor is calculated by determining the distances between all atoms pairs and the distribution of these distances forming a vector of which each bin is the sum of atom pairs in a specific range of interatomic separation,

(ii) for each of a plurality of further conformations, the corresponding multiple 3D-ACV is calculated and stored, and

(iii) principal components analysis (PCA) is preformed on each of said multiple 3D-ACVs.

12. A computer-aided method for the provision, identification and description of molecules exhibiting antibacterial activity, employing a step of molecular modelling a molecule having antibacterial activity, a step of building a combinatorial library including molecules having said antibacterial activity and a step of selecting potentially antibacterial molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors

or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said antibacterial activity .

13. A method according to claim 12 wherein the antibacterial activity is anti-S. epidermidis or anti-Corynebacterium xerosis activity.

14. A computer-aided method for the provision, identification and description of molecules exhibiting antifungal activity, employing a step of molecular modelling a molecule having antifungal activity, a step of building a combinatorial library including molecules having said antifungal activity and a step of selecting potentially antifungal molecules, wherein said method includes a step whereby the candidate molecules are filtered using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said antifungal activity or else using a static filter representing a plurality of descriptors.

15. A computer-aided method for the provision, identification and description of molecules exhibiting antibiotic activity, employing a step of molecular modelling a molecule having antibiotic activity, a step of building a combinatorial library including molecules having said antibiotic activity and a step of selecting

potentially antibiotic molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said antibiotic activity.

16. A computer-aided method for the provision, identification and description of molecules exhibiting anti-viral activity, employing a step of molecular modelling a molecule having anti-viral activity, a step of building a combinatorial library including molecules having said anti-viral activity and a step of selecting potentially anti-viral molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said anti-viral activity.

17. A computer-aided method for the provision, identification and description of molecules exhibiting anti-parasitic activity, employing a step of molecular modelling a molecule having anti-parasitic activity, a step of building a combinatorial library including molecules having said anti-parasitic activity and a step

of selecting potentially anti-parasitic molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said anti-parasitic activity .

18. A computer-aided method for the provision, identification and description of molecules exhibiting immunomodulatory, employing a step of molecular modelling a molecule having immunomodulatory activity, a step of building a combinatorial library including molecules having said immunomodulatory activity and a step of selecting potentially immunomodulatory molecules, wherein said method includes a step whereby the candidate molecules are filtered or using a static filter representing a plurality of descriptors or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said immunomodulatory activity .

19. A computer-aided method according to claim 1 wherein the combinatorial library building step comprises building a combinatorial peptide library.

20. A computer-aided method according to claim 1 wherein the combinatorial library building step comprises

building a combinatorial peptoid library.

21. A computer-aided method of designing molecules exhibiting antibacterial activity, the method comprising the following steps:

1) producing a learning set of molecules including molecules known to exhibit antibacterial activity ("active molecules") and molecules known not to exhibit antibacterial activity ("inactive molecules");

2) determining the values of a plurality of descriptors of said learning set of molecules;

3) from said values deriving one or more criteria associating descriptor values with antibacterial activity, said criteria including at least one static criterion and at least one dynamic criterion;

4) generating a plurality of candidate molecules;

5) subjecting the candidate molecules to said static criteria, and disregarding candidate molecules which do not meet said static criteria;

6) subjecting the candidate molecules to said dynamic criterion, and disregarding candidate molecules which do not meet said dynamic criteria;

7) synthesising and testing the remaining candidate molecules to determine whether said remaining candidate molecules have antibacterial activity.

22. A computer-aided method according to claim 21 wherein the learning set is comprised on the one hand of

antibacterial peptides and on the other of inactive peptides known to be devoid of said antibacterial activity.

23. A computer-aided method according to claim 21 wherein the synthesised molecule is a peptide.

24. A computer aided method according to claim 21 wherein the synthesised molecule is a peptoid.

25. A computer-aided method of designing molecules exhibiting anti-S. epidermidis or anti-Corneybacterium xerosis activity, the method comprising the following steps:

1) producing a learning set of molecules including molecules known to exhibit anti-S. epidermidis or anti-Corneybacterium xerosis activity ("active molecules") and molecules known not to exhibit anti-S. epidermidis or anti-Corneybacterium xerosis activity ("inactive molecules");

2) determining the values of a plurality of descriptors of said learning set of molecules;

3) from said values deriving one or more criteria associating descriptor values with anti-S. epidermidis or anti-Corneybacterium xerosis activity, said criteria including at least one static criterion and at least one dynamic criterion;

4) generating a plurality of candidate molecules;

5) subjecting the candidate molecules to said static criteria, and disregarding candidate molecules which do not meet said static criteria;

6) subjecting the candidate molecules to said dynamic criterion, and disregarding candidate molecules which do not meet said dynamic criteria;

7) synthesising and testing the remaining candidate molecules to determine whether said remaining candidate molecules have anti-S. epidermidis or anti-Corneybacterium xerosis activity.

26. A computer aided method according to claim 25 wherein the learning set is comprised on the one hand of peptides known to exhibit anti- Corneybacterium xerosis or S. epidermidis activity and on the other of inactive peptides known to be devoid of said anti- Corneybacterium xerosis or S. epidermidis activity.

27. A computer aided method according to claim 25 wherein the synthesised molecule is a peptide.

28. A computer aided method according to claim 25 wherein the synthesised molecule is a peptoid.

29. A computer-aided method of designing molecules exhibiting anti-fungal activity, the method comprising the following steps:

1) producing a learning set of molecules including

molecules known to exhibit anti-fungal activity ("active molecules") and molecules known not to exhibit anti-fungal activity ("inactive molecules");

2) determining the values of a plurality of descriptors of said learning set of molecules;

3) from said values deriving one or more criteria associating descriptor values with anti-fungal activity, said criteria including at least one static criterion and at least one dynamic criterion;

4) generating a plurality of candidate molecules;

5) subjecting the candidate molecules to said static criteria, and disregarding candidate molecules which do not meet said static criteria;

6) subjecting the candidate molecules to said dynamic criterion, and disregarding candidate molecules which do not meet said dynamic criteria;

7) synthesising and testing the remaining candidate molecules to determine whether said remaining candidate molecules have anti-fungal activity.

30. A computer aided method according to claim 29 wherein the learning set is comprised on the one hand of anti-fungal peptides and on the other of inactive peptides known to be devoid of said anti-fungal activity.

31. A computer aided method according to claim 29 wherein the synthesised molecule is a peptide.

32. A computer aided method according to claim 29 wherein the synthesised molecule is a peptoid.

33. A computer-aided method of designing molecules exhibiting anti-viral activity, the method comprising the following steps:

1) producing a learning set of molecules including molecules known to exhibit anti-viral activity ("active molecules") and molecules known not to exhibit anti-viral activity ("inactive molecules");

2) determining the values of a plurality of descriptors of said learning set of molecules;

3) from said values deriving one or more criteria associating descriptor values with anti-viral activity, said criteria including at least one static criterion and at least one dynamic criterion;

4) generating a plurality of candidate molecules;

5) subjecting the candidate molecules to said static criteria, and disregarding candidate molecules which do not meet said static criteria;

6) subjecting the candidate molecules to said dynamic criterion, and disregarding candidate molecules which do not meet said dynamic criteria;

7) synthesising and testing the remaining candidate molecules to determine whether said remaining candidate molecules have anti-viral activity.

34. A computer aided method according to claim 33

wherein the learning set is comprised on the one hand of anti-viral peptides and on the other of inactive peptides known to be devoid of said anti-viral activity.

35. A computer aided method according to claim 33 wherein the synthesised molecule is a peptide.

36. A computer aided method according to claim 33 wherein the synthesised molecule is a peptoid.

37. A computer-aided method of designing molecules exhibiting anti -parasitic activity, the method comprising the following steps:

1) producing a learning set of molecules including molecules known to exhibit anti -parasitic activity ("active molecules") and molecules known not to exhibit anti -parasitic activity ("inactive molecules");

2) determining the values of a plurality of descriptors of said learning set of molecules;

3) from said values deriving one or more criteria associating descriptor values with anti -parasitic activity, said criteria including at least one static criterion and at least one dynamic criterion;

4) generating a plurality of candidate molecules;

5) subjecting the candidate molecules to said static criteria, and disregarding candidate molecules which do not meet said static criteria;

6) subjecting the candidate molecules to said dynamic

criterion, and disregarding candidate molecules which do not meet said dynamic criteria;

7) synthesising and testing the remaining candidate molecules to determine whether said remaining candidate molecules have anti -parasitic activity.

38. A computer aided method according to claim 37 wherein the learning set is comprised on the one hand of anti -parasitic peptides and on the other of inactive peptides known to be devoid of said anti -parasitic activity.

39. A computer aided method according to claim 37 wherein the synthesised molecule is a peptide.

40. A computer aided method according to claim 37 wherein the synthesised molecule is a peptoid.

41. A computer-aided method of designing molecules exhibiting immunomodulatory activity, the method comprising the following steps:

1) producing a learning set of molecules including molecules known to exhibit immunomodulatory activity ("active molecules") and molecules known not to exhibit immunomodulatory activity ("inactive molecules");

2) determining the values of a plurality of descriptors of said learning set of molecules;

3) from said values deriving one or more criteria

associating descriptor values with immunomodulatory activity, said criteria including at least one static criterion and at least one dynamic criterion;

4) generating a plurality of candidate molecules;

5) subjecting the candidate molecules to said static criteria, and disregarding candidate molecules which do not meet said static criteria;

6) subjecting the candidate molecules to said dynamic criterion, and disregarding candidate molecules which do not meet said dynamic criteria;

7) synthesising and testing the remaining candidate molecules to determine whether said remaining candidate molecules have immunomodulatory activity.

42. A computer aided method according to claim 41 wherein the learning set is comprised on the one hand of immunomodulatory peptides and on the other of inactive peptides known to be devoid of said immunomodulatory activity.

43. A computer aided method according to claim 41 wherein the synthesised molecule is a peptide.

44. A computer aided method according to claim 41 wherein the synthesised molecule is a peptoid.

45. A computer aided method according to any one of the preceding claims further comprising the step of

physically generating a molecule thus selected.

46. A computer aided method according to claim 45 wherein the generated molecule is a peptide

47. A computer aided method according to claim 45 wherein the generated molecule is a peptoid.

48. A molecule exhibiting a desired behaviour obtained by the method according to claim 45.

49. A molecule according to claim 48 wherein the molecule is for use in the pharmaceutical sector.

50. A molecule exhibiting a desired behaviour obtainable by the method according to claim 45.

51. A molecule according to claim 50 wherein the molecule is for use in the pharmaceutical sector.

52. A computer aided method for producing a molecule exhibiting a desired behaviour including the steps of:

(1) carrying out the computer aided design method based according to claim 1;

(2) selecting a molecule and;

(3) synthesising the selected molecule.

53. A computer aided method according to claim 52

comprising the further step of:

(4) admixing the selected molecule with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

54. A computer aided method for producing a molecule exhibiting a desired behaviour including the steps of:

(1) carrying out the computer aided design method based according to claim 3;

(2) selecting a molecule and;

(3) synthesising the selected molecule.

55. A computer aided method for producing a peptide exhibiting a desired behaviour including the steps of:

(1) carrying out the computer aided design method based according to claim 1;

(2) selecting a peptide and;

(3) synthesising the selected peptide.

56. A computer aided method for producing a peptide exhibiting a desired behaviour including the steps of:

(1) carrying out the computer aided design method according to claim 3;

(2) selecting a peptide and;

(3) synthesising the selected peptide.

57. A computer aided method for producing a peptide exhibiting a desired behaviour including the steps of:

(1) carrying out the computer aided design method according to claim 1, wherein the combinatorial library comprises peptides;

(2) selecting a peptide and;

(3) synthesising the selected peptide.

58. A computer aided method for producing a peptide exhibiting a desired behaviour including the steps of:

(1) carrying out the computer aided design method according to claim 1, wherein the combinatorial library comprises peptoids;

(2) selecting a peptoid and;

(3) synthesising a peptoid based on the selected peptide.

59. A molecule other than a known reference molecule, which molecule exhibits a desired activity of said known reference molecule, wherein said molecule occupies a conformational space of, or very similar to at least one known reference molecule exhibiting said desired behaviour.

60. A molecule according to claim 59 wherein said desired activity is selected from: Anti-bacterial activity, anti-fungal activity, anti-viral activity, anti-parasitic activity, antibiotic activity and immunomodulatory activity.

61. A molecule other than a known reference molecule, which molecule exhibits a desired activity of said known reference molecule, which molecule exhibits the ranges of variation of static descriptors identical or very similar to ranges of variation of static descriptors of at least one known reference molecule exhibiting said desired behaviour.

62. A molecule according to claim 61 wherein said desired activity is selected from: Anti-bacterial activity, anti-fungal activity, anti-viral activity, anti-parasitic activity, antibiotic activity and immunomodulatory activity.

63. A molecule other than a known reference molecule, which molecule exhibits a desired activity of said known reference molecule, wherein said molecule occupies a conformational space identical or very similar to the conformational space of at least one known reference molecule exhibiting said desired behaviour, and in that it exhibits ranges of variation of static descriptors identical or very similar to the ranges of variation of static descriptors of at least one known reference molecule exhibiting said desired behaviour.

64. A molecule according to claim 63 wherein said desired activity is selected from: Anti-bacterial

activity, anti-fungal activity, anti-viral activity, anti-parasitic activity, antibiotic activity and immunomodulatory activity.

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